Matching the High Momentum Modes in a Truncated Determinant Algorithm

A. Duncan[a],E. Eichten*[b] and H. Thacker[c]

[a]Dept. of Physics and Astronomy, Univ. of Pittsburgh, Pittsburgh, PA 15260

[b]Fermilab, P.O. Box 500, Batavia, IL 60510

[c]Dept.of Physics, University of Virginia, Charlottesville, VA 22901

Within a truncated determinant algorithm, two alternatives are discussed for including systematically the remaining ultraviolet modes. Evidence is presented that these modes are accurately described by an effective action involving only small Wilson loops.

1. Introduction

Because QCD in four dimensions is renormalizable, not super-renormalizable, the fluctuations of the fermion determinant are significant at all physical scales. Fortunately the short distance behaviour of QCD is very well understood. In particular, we know that for sufficiently high momentum scales this physics should be accurately described by an improved gauge action.

In the truncated determinant algorithm[1], the fermion determinant is separated into two pieces

$$\ln \det H = [\mathrm{Tr} \ln H]_{low\ \lambda} + [\mathrm{Tr} \ln H]_{high\ \lambda} \qquad (1)$$

where the lowest $n_{\rm cut}$ eigenvalues are directly calculated and included in the Monte Carlo updating procedure. The higher eigenvalues can be included in the Monte Carlo by some approximation that matches onto the low eigenvalue results without gaps or double counting, is controlled and becomes exact in the continuum limit.

Two numerical methods suggest themselves for calculating the high eigenvalues: (1)The multiboson approach of Lüscher[2]. (2)Using a small number of gauge loops to model the determinant as proposed by Sexton and Weingarten [3], and Irving and Sexton [4].

*Presenter

2. Matching onto the Multiboson Method

One method to compute the high eigenvalues which is guaranteed to succeed is the multiboson approach of Lüscher[2]. Define

$$P_{eff}(U) \equiv [\det(\mathrm{D} + \mathrm{m})]^{n_f} \exp\left(-S_g(U)\right) \qquad (2)$$

and

$$H = \gamma_5(\mathrm{D} + \mathrm{m})/[\mathrm{c_m}(8 + \mathrm{m})] \quad (c_m \geq 1) \qquad (3)$$

where c_m is chosen so that the eigenvalues of H are in the interval $(-1, 1)$. Lüscher chooses a sequence of polynomials $P_n(s)$ of even degree n such that

$$\lim_{n\to\infty} P_n(s) = 1/s \quad \text{for all } 0 < s \leq 1 \qquad (4)$$

then for $n_f = 2$

$$\det H^2 = \lim_{n\to\infty} [\det P_n(H^2)]^{-1} \qquad (5)$$

Choose polynomials such that complex roots $z_1 \ldots z_n$ come in complex conjugate pairs (non real) so that $\sqrt{z} = \mu + i\nu$. Then

$$\det H^2 = \lim_{n\to\infty} \prod_{k=1}^{n} \det[(H - \mu_k)^2 + \nu_k^2]^{-1} \qquad (6)$$

Hence we can write

$$P_{eff}(U) = \lim_{n\to\infty} \frac{1}{Z_b} \int D\phi D\phi^\dagger \exp -(S_g + S_b) \qquad (7)$$

where the bosonic action is given by

$$S_b = \sum_{k=1}^{n} \sum_{x} |(H - \mu_k)\phi_k(x)|^2 + \nu^2 |\phi_k(x)|^2. \quad (8)$$

Lüscher used Chebyshev polynomials to estimate how many boson fields (n_b) are required to represent the original action to a fixed accuracy in the range ($\epsilon < s \leq 1$) The error is given by[2]:

$$|R(s)| \leq 2(\frac{1-\sqrt{\epsilon}}{1+\sqrt{\epsilon}})^{n_b+1}. \quad (9)$$

Therefore, the convergence is exponential with rate $2\sqrt{\epsilon}$ as $n_b \to \infty$.

A practical problem with this multiboson method is that it requires an increasingly large number of boson fields as the quark mass becomes lighter. As $m_q \to 0$, we must take $\epsilon \to 0$, but to obtain a fixed level of accuracy we must hold $2\sqrt{\epsilon}n_b$ fixed and hence n_b increases without bound.

However the multiboson method matches nicely onto the calculation of low eigenvalues. This was first suggested by Alexandrou et.al.[5]. In the truncated determinant method, the cutoff ϵ for the multiboson method is set by the highest eigenvalue of H^2 which is explicitly included in the low end calculations. Hence it does not explode as the quark mass goes to zero. The combination of methods remain accurate for all quark masses. For example, for $\beta = 5.9$ on a 12^3x24 lattice with direct inclusion of the lowest 100 eigenvalues, the associated cutoff for the multiboson simulation of the high eigenvalues is $\sqrt{\epsilon} \approx 0.035$ independent of the light quark mass.

Furthermore, the error associated with the inaccurate behaviour of the polynomial fit in the range $0 < s < \epsilon$ can be corrected as low eigenvalues are computed for every configuration update. We obtain a reweighting term,

$$\Delta S_b = \sum_{i=1}^{n_{\rm cut}} \ln(\lambda_i^2 P(\lambda_i^2)) \quad (10)$$

which can be included to eliminate errors in the region $0 < s \leq \epsilon$.

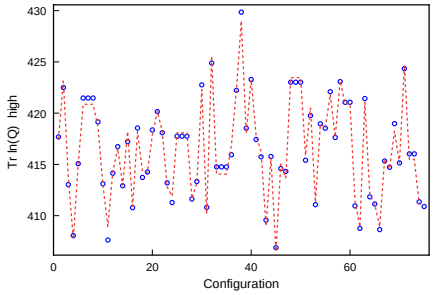

Figure 1. Comparison of $(\mathrm{Tr}\ln H)_{\mathrm{high}\lambda}$ (dashed line) and best fit (up to 6 links) effective gauge action (open circles) for 75 gauge configurations.

3. Matching onto Small Loops

Using the multiboson method for the high end of the determinant satisfies all our requirements and completes the algorithm. However it may be possible to reduce the total required computations even further using a more physical approach to the high eigenvalues. Consider how many of the high eigenvalues actually have physical information and are not just lattice artifacts. For example, for a 12^3x24 lattice with $\beta = 5.9$ and $\kappa = .1587$ there are 497,664 total eigenvalues of the Wilson-Dirac operator; while for a high energy cutoff of 1 GeV we have approximately 1500 eigenvalues (0.3%). For a fixed volume V and quark mass m_q a decreasing fraction of the eigenvalues are below a fixed physical scale as $\beta \to \infty$. Therefore, most of the range of large s fit in Lüscher's multiboson method is physically unimportant.

This suggests a more physically motivated method for dealing with the high eigenvalue part of the fermion determinant in which one approximates the ultraviolet contribution to the quark determinant with an effective gauge action:

$$[\mathrm{Tr}\ln H]_{high\ \lambda} \approx \sum_{i=0}^{i_{max}} \alpha_i L_i \quad (11)$$

where each L_i is a set of gauge links which form a closed path. The natural expansion is in the number of links. For zero links L_0 is just a constant, for four links we have a plaquette, and six links give the three terms found in considerations

of improved gauge actions [6].

This idea was studied in detail by Irving and Sexton[4]. These studies were done on a 6^4 lattice at $\beta = 5.7$ with Hybrid Monte-Carlo full QCD simulations (with a heavy sea quark). Their results were rather discouraging. It was hard to get a good approximation to the determinant with a closed set of loops and they needed large loops to even approach a reasonable fit[4].

There are however two important differences between their study and our situation. First, they simulated the *whole determinant*, while here we only need to approximate the eigenvalues above some cutoff. Hence we would expect the small loops to dominate at least for sufficiently high cutoff. Second, they used an approximate procedure to estimate stochastically the logarithm of the determinant needed, while we are exactly computing all eigenvalues for this study. It turns out that these differences are critical, as using approximately the same lattices (and with even lighter quarks) we find an excellent approximation to the high end with only small loops.

We generated a set of 75 configurations on a 6^4 lattice at $\beta = 5.7$ and $\kappa = .1685$. We included the lowest 30 eigenvalues (which corresponds to a physical cutoff of approximately $\simeq$350 Mev) in the Monte Carlo accept/reject step in the generation of these independent configurations.

Considering only the high eigenvalues, an excellent fit to the fluctuations is obtained including four and six link closed loops. The variance of the fit is 0.265. The comparison between the fluctuations in the exact (S_t) and approximate (S_a) actions for the high eigenvalue piece is shown in Fig 1. As expected, if only the plaquette term is included the variance is larger (2.25) and we must move the low eigenvalue cutoff to $N = 50$ ($\approx$ 700 MeV) to reduce the variance below one. The results for various cutoffs and terms included are shown in Table 1.

The linear combination (.46,-.55,.04,.70,.03) for (plaquette,rectangle,chair,polygon,wilsonline) gives the best fit to the high eigenvalues of the quark determinant (with $n_{\rm cut} = 30$). The configuration to configuration variations of the individual 6-link terms are highly correlated. This is to be expected since these three terms are not independent.

n_λ cut	λ (MeV)	4 links	6 links (with WL)
0	0	4.98	1.074 (0.835)
$\pm$15	340	2.25	0.2652 (0.233)
$\pm$50	700	0.940	0.0564 (0.0491)
$\pm$250	1,210	0.0733	0.0695 (0.0641)
$\pm$1250	2,220	0.138	0.0198 (0.0180)

Table 1
Variance ($< (S_a - S_t)^2 >^{1/2}$) of fit to high eigenvalues of the quark determinant by various sets of small gauge loops (WL denotes a Wilson line).

The coefficients of the effective action should be independent of the physical volume with other physical parameters held constant. We are repeating this study for an (8^4) lattice. The preliminary study on 41 configurations gives the same fit parameters within the statistical accuracy. With $n_{\rm cut} = 120$ ($\lambda \approx 350\,$MeV) the variance is 0.52.

Although more study is required, this second method looks very attractive for dealing with the high end of the fermion determinant in full QCD with light dynamical quarks. Simulations would be performed by including the predetermined effective gauge action S_a in the gauge updates and computing the infrared part of the determinant as in the truncated determinant simulations.

REFERENCES

1. A. Duncan, E. Eichten and H. Thacker, hep-lat 9806020; A. Duncan, these proceedings.
2. M. Lüscher, Nucl. Phys. **B418**, 637 (1994).
3. J. C. Sexton and D. H. Weingarten, Phys. Rev. **D55** 4025 (1997).
4. A. C. Irving and J. C. Sexton, Phys. Rev. **D55** 5456 (1997); A.C. Irving, J.C. Sexton and E. Cahill,hep-lat/9708004.
5. C. Alexandrou, A. Borrelli, Ph. de Forcrand, A. Galli, and F. Jegerlehner, Nucl. Phys. **B456**, 296 (1995).
6. M. Lüscher and P. Weisz, Phys. Lett. **158B** 250 (1985), and references therein.